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Minimal irreversible quantum mechanics: The mixed states and the diagonal singularity

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A formalism for minimal irreversible quantum mechanics is extended from pure states to mixed states. In the latter case the problem of their diagonal singularity is explained and solved. In addition to the pure and mixed states of the usual approach, more general states are obtained. The Friedrichs model is studied. Decoherence is found and decoherence characteristic times are computed. [S1050-2947(98)03505-7]

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I. INTRODUCTION

The diagonal singularity of operators in large quantum systems, having continuous energies, was discovered by van Hove [1–4]. At the same time, Prigogine and co-workers [5–8] emphasized the importance of states with diagonal singularity in nonequilibrium statistical physics. A key point in the approach to this problem is the projection onto the diagonal part of states, for which the Pauli master equation is obtained through the thermodynamic limit, because direct calculation on the continuous spectrum gives rise to divergencies. In recent papers Antoniou *et al.* [9–11] developed a formulation of quantum theory that allows a natural definition of states and observables with diagonal singularity, projections onto the diagonal and off-diagonal parts, generalized traces of states, mean values of observables, and the construction of a continuous orthonormal basis for states and observables.

In this formalism, the expectation value $\langle O\rangle_\rho$ of an observable O in the state ρ is represented by the action of a functional $(\dot{\rho}|$ on an operator $|O)$ $[\langle O\rangle_\rho=\rho[O]=(\rho|O)]$, which opens the possibility, by the rigging of the space of observables, to obtain generalized spectral decompositions with complex eigenvalues of the Liouville–Von Neumann operator with a dominant contribution in the approach to equilibrium of macroscopic systems or in the decay processes of microscopic systems. We have used this kind of formalism to study the evolution of an oscillator coupled with a field in Ref. [12].

On the other hand, for the Friedrichs model, Petrosky, Prigogine, and Tasaki [13] obtained explicit formulas of generalized eigenvectors of the Hamiltonian with complex eigenvalues, using a perturbative scheme based on a time ordering rule. The eigenvectors for the Friedrichs model were constructed by Sudarshan, Chiu, and Gorini [14] using analytic continuation techniques. Later, Antoniou and Prigogine [15] pointed out that these generalized eigenvectors acquire meaning in suitable rigged Hilbert spaces, associated with Hardy class functions, introduced by Bohm [16–19]. We have developed these ideas for pure states in Ref. [20]. The aim of this work is to extend the results of Ref. [20] to the mixed states and to apply the formalism of quantum systems with diagonal singularity to the Friedrichs model, which is a prototype model for the decay problem in quantum mechanics, and through this approach clarify the role of the complex spectral decomposition in the description of the time evolution of unstable states of quantum systems.

In Sec. II we present a brief description of the formalism developed by Antoniou *et al.* [9–11], and already used by us in Ref. [12], for quantum systems with diagonal singularities. We give the definitions of states and observables, the generalized definition of the trace for the states, the mean values for the observables, and the time evolution. The weak limit for $t\to\infty$ of the time evolution turns out to be a diagonal state. Therefore decoherence appears as a weak limit. This is a first manifestation that the formalism already contains the base for irreversibility. States and observables with diagonal singularity, time evolution, and asymptotic states are discussed in Sec. III for the Friedrichs model. In Sec. IV we endow the set of observables and states with analyticity properties that break the time symmetry, as in Ref. [20], and they allow us to formulate a generalized spectral decomposition with complex eigenvalues and to compute decoherence times. In Sec. V we state our main conclusions.

II. STATES AND OBSERVABLES WITH DIAGONAL SINGULARITY

A. The usual formalism and its problems

Let us consider a system with a Hamiltonian having a continuous spectrum

$$H=\int_0^\infty dE E|E\rangle\langle E|, \tag{1}$$

$|E\rangle$ ($\langle E|$) being generalized right (left) eigenvectors of H with eigenvalue E.

The time evolution of a pure state is given by

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$$|\Psi_t\rangle = e^{-iHt}|\Psi_0\rangle = \int_0^\infty dE|E\rangle\Psi_t(E),$$

$$\Psi_t(E) = e^{-iEt}\langle E|\Psi_0\rangle. \tag{2}$$

The wave function $\Psi_t(E)$ has an oscillatory time dependence, and therefore it does not have a well-defined limit when $t\to\infty$. However, it is possible to obtain a well-defined limit for the mean value of any observable, within a space of observables $\mathcal{O}$, represented by self-adjoint operators with a form that generalizes the one of H; precisely,

$$O = \int_0^\infty dE O_E|E\rangle\langle E| + \int_0^\infty dE\int_0^\infty dE' O_{EE'}|E\rangle\langle E'|. \tag{3}$$

We explicitly include a diagonal singularity and assume that $O_E = O_E^*$ and $O_{EE'} = O_{E'E}^*$ are ordinary functions. The Hamiltonian (1) is of the form given in Eq. (3) with $O_E = E$ and $O_{EE'} = 0$.

The time evolution of the mean value of O in the pure state (2) is given by

$$\begin{aligned}\langle O\rangle_t &= \langle\Psi_t|O|\Psi_t\rangle\\ &= \int dE\langle E|\Psi_0\rangle\langle\Psi_0|E\rangle O_E\\ &\quad + \int\int dE dE' e^{-i(E-E')t}\langle E|\Psi_0\rangle\langle\Psi_0|E'\rangle O_{E'E}.\end{aligned} \tag{4}$$

Under mild conditions [for example, if $g_0(E,E') = \langle E|\Psi_0\rangle\langle\Psi_0|E'\rangle O_{E'E}$ is a Schwartz function in $[0,\infty)\times[0,\infty)$, see Appendix], the last term in Eq. (4) goes to zero when $t\to\infty$, and we obtain

$$\lim_{t\to\infty}\langle O\rangle_t = \int dE\langle E|\Psi_0\rangle\langle\Psi_0|E\rangle O_E. \tag{5}$$

If we consider a mixture, i.e., a set of normalized state vectors $\Psi^{(\alpha)}$ with probabilities $p^{(\alpha)}$ ($\Sigma_\alpha p^{(\alpha)} = 1$, $p^{(\alpha)} \geqslant 0$), the time-dependent density operator is

$$\hat{\rho}_t = \sum_\alpha p^{(\alpha)}|\Psi_t^{(\alpha)}\rangle\langle\Psi_t^{(\alpha)}|, \quad |\Psi_t^{(\alpha)}\rangle = e^{-iHt}|\Psi_0^{(\alpha)}\rangle,$$

$$\mathrm{Tr}\hat{\rho}_t = 1.$$

Therefore, we have

$$\langle E|\hat{\rho}_t|E'\rangle = e^{-i(E-E')t}\sum_\alpha p^{(\alpha)}\langle E|\Psi_0^{(\alpha)}\rangle\langle\Psi_0^{(\alpha)}|E'\rangle,$$

with no well-defined limit for $t\to\infty$.

The mean value in the mixed state of an observable represented by an operator of the form given by Eq. (3) is

$$\begin{aligned}\langle O\rangle_t &= \mathrm{Tr}(\hat{\rho}_t O)\\ &= \int dE\sum_\alpha p^{(\alpha)}\langle E|\Psi_0^{(\alpha)}\rangle\langle\Psi_0^{(\alpha)}|E\rangle O_E\\ &\quad + \int\int dE\, dE' e^{-i(E-E')t}\sum_\alpha p^{(\alpha)}\langle E|\Psi_0^{(\alpha)}\rangle\\ &\quad \times\langle\Psi_0^{(\alpha)}|E'\rangle O_{E'E}.\end{aligned}$$

If the conditions given in the Appendix are fulfilled, the limit $t\to\infty$ of the last expression is well defined:

$$\lim_{t\to\infty}\langle O\rangle_t = \int dE\sum_\alpha p^{(\alpha)}\langle E|\Psi_0^{(\alpha)}\rangle\langle\Psi_0^{(\alpha)}|E\rangle O_E. \tag{6}$$

Let us present some problems with this formalism to motivate the different approach we shall present in Sec. II B.

(i) As Eq. (6) gives the final mean value of the observable O, we may try to find a density operator

$$\hat{\rho}_\infty = \int\int dE\, dE'(\hat{\rho}_\infty)_{EE'}|E\langle E'|,$$

such that $\lim_{t\to\infty}\langle O\rangle_t = \mathrm{Tr}(\hat{\rho}_\infty O)$, which would imply

$$\begin{aligned}&\int dE\sum_\alpha p^{(\alpha)}\langle E|\Psi_0^{(\alpha)}\rangle\langle\Psi_0^{(\alpha)}|E\rangle O_E\\ &\quad = \int dE(\hat{\rho}_\infty)_{EE}O_E + \int\int dE\, dE'(\hat{\rho}_\infty)_{EE'}O_{EE'}.\end{aligned} \tag{7}$$

But there is no regular function $(\hat{\rho}_\infty)_{EE'}$ satisfying the previous equation for arbitrary O_E and $O_{EE'}$.

(ii) The state corresponding to a well-defined value E of the energy is represented by the generalized eigenvector $|E\rangle$ of the Hamiltonian. However, $|E\rangle$ is not in the space of normalized vectors. Expressions such as $\langle E|E\rangle$ or $\langle E|H|E\rangle$ are not well defined, since essentially they are products of distributions.

B. The functional approach

It is possible to eliminate the difficulties presented at the end of Sec. II A with an extended definition of the states as functionals acting on the operators representing observables. If the observable O is represented by a self-adjoint operator having diagonal singularity, as is the case for expression (3), the state ρ of the system can be represented in similar fashion by two ordinary functions ρ_E and $\rho_{EE'}$, such that the mean value $\langle O\rangle_\rho$ of the observable is given by

$$\langle O\rangle_\rho = (\rho|O) = \int dE\rho_E^* O_E + \int\int dE\, dE'\rho_{EE'}^* O_{EE'}. \tag{8}$$

This definition is based in the following physical arguments: we do not measure the quantum states directly, we only measure the mean values of observables in states. Only in order to obtain these values we must define the notion of state. Therefore the state is just a functional over the space of observables $\rho[O]=(\rho|O)$, such that $\rho_E^*\equiv\rho[|E\rangle\langle E|]$ and $\rho_{EE'}^*\equiv\rho[|E\rangle\langle E'|]$.

The mean value $\langle O\rangle_\rho$ is real if

$$\rho_E^*=\rho_E, \quad \rho_{EE'}^*=\rho_{E'E}. \tag{9}$$

We also have $\langle I\rangle_\rho=\langle\int dE|E\rangle\langle E|\rangle_\rho=(\rho|I)=1$ if

$$\int_0^\infty dE\rho_E^*=1. \tag{10}$$

Moreover, ρ_E^* can be interpreted as the probability density of the system of being in the generalized state vector $|E\rangle$, and we should have

$$\rho_E^*\geqslant 0. \tag{11}$$

Therefore, the states ρ are represented by functionals of the space $\mathcal{O}'$ acting on the space of operators $\mathcal{O}$ representing observables. These states can be expressed in terms of the functionals $(E|$ and $(EE'|$, defined by the relations

$$(E|O)=O_E, \quad (EE'|O)=O_{EE'}.$$

From these expressions we obtain

$$(E|E')=\delta(E-E'), \quad (E|E'E'')=0,$$

$$(EE'|E''E''')=\delta(E-E'')\delta(E'-E'''), \quad (EE'|E'')=0, \tag{12}$$

where

$$|E)\equiv|E\rangle\langle E|, \quad |EE')\equiv|E\rangle\langle E'|. \tag{13}$$

After these introductory reasonings let us give some definitions. Using (13), we can give the following ket expression for an operator $|O)$ representing an observable O with diagonal singularity:

$$|O)=\int dEO_E|E)+\int\int dE\, dE'O_{EE'}|EE'). \tag{14}$$

If $O_E=O_E^*$, $O_{EE'}=O_{E'E}^*$ are ordinary functions, we will say that $O\in\mathcal{O}$, *the space of observables*.

Using Eq. (12), the following bra expression can be given for a functional $(\rho|$ representing a state ρ:

$$(\rho|=\int dE\rho_E^*(E|+\int\int dE\, dE'\rho_{EE'}^*(EE'|. \tag{15}$$

If $\rho_E=\rho_E^*\geqslant 0$, $\rho_{EE'}=\rho_{E'E}^*$, and $\int_0^\infty dE\rho_E^*=1$, where ρ_E and $\rho_{EE'}$ are ordinary functions,[1] we will say that $\rho\in\mathcal{S}$, *the space of the states*. Obviously $\mathcal{S}\subset\mathcal{O}'$, the dual space of $\mathcal{O}$.

Using Eqs. (12), (14), and (15) we can easily prove, as expected, that

$$\langle O\rangle_\rho=(\rho|O)=\int dE\rho_E^*O_E+\int\int dE\, dE'\rho_{EE'}^*O_{EE'}. \tag{16}$$

Additional conditions should be satisfied by ρ_E^*, $\rho_{EE'}^*$, O_E, and $O_{EE'}$, so that the integrals in Eq. (16) are well defined. These conditions depend on the class of observables and states of the model for which we expect well-defined mean values.[2] For example, if the energy and its dispersion are to be well defined, ρ_E^* should satisfy $(\rho|H^n)=\int dE\rho_E^*E^n<\infty$. Eventually, the conditions stated in the Appendix will also be imposed, so that the time evolution of the system has a well-defined limit for $t\to\infty$.

Conditions (9) and (10) can be written as

$$(\rho|O)=(\rho|O)^* \quad \text{if} \quad O^\dagger=O, \tag{17}$$

$$(\rho|I)=(\rho|\int dE|E)=1. \tag{18}$$

Expression (18) can be considered as a *generalization of the concept of trace for the state functional* ρ.

In the functional approach, the time evolution of the states is determined by an operator $\mathbb{U}_t$ acting on ρ and defined by

$$(\rho_t|O)=(\mathbb{U}_t\rho_0|O)=(\rho_0|\mathbb{U}_t^\dagger O)=(\rho_0|e^{i\mathbb{L}^\dagger t}O)$$
$$=(\rho_0|e^{iH^\dagger t}Oe^{-iHt}), \tag{19}$$

which also gives the relation between the Schrödinger and Heisenberg pictures.

The generalized Liouville–Von Neumann equation can be deduced from the previous equation

$$-i\frac{d}{dt}(\rho_t|=(\mathbb{L}\rho_t|=(\rho_t|\mathbb{L}^\dagger, \quad \mathbb{L}^\dagger O\equiv H^\dagger O-OH. \tag{20}$$

The bras $(E|$ and $(EE'|$ [kets $|E)$ and $|EE')$] are generalized left (right) eigenvectors of the Liouville–Von Newmann superoperator $\mathbb{L}^\dagger$

$$(E|\mathbb{L}^\dagger=0, \quad \mathbb{L}^\dagger|E)=0, \quad (EE'|\mathbb{L}^\dagger=(E-E')(EE'|,$$
$$\mathbb{L}^\dagger|EE')=(E-E')|EE'),$$

and therefore

$$(\rho_t|=\int dE(\rho_t)_E^*(E|+\int\int dEdE'(\rho_t)_{EE'}^*(EE'|$$
$$=\int dE(\rho_0)_E^*(E|+\int\int dE\, dE'(\rho_0)_{EE'}^*$$
$$\times e^{i(E-E')t}(EE'|. \tag{21}$$

[1]In some very exceptional cases we will allow that $\rho_E^*=\delta(E-\tilde{E})$.

[2]However, the toy model with the Hamiltonian given by Eq. (1), in which we based our presentation of the functional approach, does not allow us to discuss further the characteristics of the measurement and preparation apparatuses. In Ref. [12], we consider $\mathcal{O}$ as the space of intensive observables to describe the thermodynamic limit of the Friedrichs model.

The time evolution of the mean value of an observable is

$$\langle O\rangle_{\rho_t}=\int dE(\rho_0)^*_E O_E + \int\int dE dE'(\rho_0)^*_{EE'} e^{i(E-E')t} O_{EE'} . \quad (22)$$

It is interesting to point out that the formalism defined above already contains the usual approach of quantum mechanics with its pure and mixed states.

(i) Consider a *pure state*, represented by a normalized vector

$$|\Psi\rangle=\int dE\Psi(E)|E\rangle, \quad \langle\Psi|\Psi\rangle=\int dE\Psi(E)^*\Psi(E)=1. \quad (23)$$

Using the standard formalism for an observable O with diagonal singularity as in Eq. (3), we obtain

$$\langle O\rangle_\Psi=\langle\Psi|O|\Psi\rangle = \int dE\Psi(E)^*\Psi(E)O_E + \int\int dE dE'\Psi(E)^*\Psi(E')O_{EE'} \quad (24)$$

(of course, the first term of the right-hand side would be absent if the observable did not have diagonal singularity). In the functional approach, the pure state is represented by the functional

$$(\rho_{\text{pure}}|\equiv\int dE\Psi(E)^*\Psi(E)(E| + \int\int dE dE'\Psi(E)^*\Psi(E')(EE'|. \quad (25)$$

It is easy to verify, from the definition (25), that $(\rho_{\text{pure}})^*_E=(\rho_{\text{pure}})_E\geqslant 0$ and $(\rho_{\text{pure}})^*_{EE'}=(\rho_{\text{pure}})_{E'E}$, and therefore $(\rho_{\text{pure}}|$ satisfies Eqs. (9) and (11). Condition (10) is also verified by $(\rho_{\text{pure}}|$ as a consequence of the normalization (23) of the vector $|\Psi\rangle$. The functional $(\rho_{\text{pure}}|$ acting on $|O)$ gives

$$(\rho_{\text{pure}}|O)=\langle\Psi|O|\Psi\rangle,$$

as expected.

(ii) If the state is a *mixture*, represented in the standard formalism by a density operator

$$\hat\rho=\sum_\alpha p^{(\alpha)}|\Psi^{(\alpha)}\rangle\langle\Psi^{(\alpha)}|,$$

the mean value of an observable O is given by

$$\langle O\rangle=\text{Tr}(\hat\rho O) = \int dE\sum_\alpha p^{(\alpha)}\langle E|\Psi^{(\alpha)}\rangle\langle\Psi^{(\alpha)}|E\rangle O_E + \int\int dE\ dE'\sum_\alpha p^{(\alpha)}\langle E|\Psi^{(\alpha)}\rangle\langle\Psi^{(\alpha)}|E'\rangle O_{EE'} .$$

This mixed state can also be described using the functional approach, if we define

$$(\rho_{\text{mix}}|\equiv\int dE\sum_\alpha p^{(\alpha)}\langle E|\Psi^{(\alpha)}\rangle\langle\Psi^{(\alpha)}|E\rangle(E| + \int\int dE\ dE'\sum_\alpha p^{(\alpha)}\langle E|\Psi^{(\alpha)}\rangle\langle\Psi^{(\alpha)}|E'\rangle(EE'|. \quad (26)$$

It is easy to verify that

$$(\rho_{\text{mix}}|O)=\text{Tr}(\hat\rho O), \quad (\rho_{\text{mix}}|I)=1, \quad (\rho_{\text{mix}}|O)=(\rho_{\text{mix}}|O)^*.$$

As we see from Eqs. (25) and (26), *the functional representation of pure or mixed states satisfies* $\rho_E=\rho_{EE}$, *and therefore the diagonal and the regular parts of* $(\rho_{\text{pure}}|$ *or* $(\rho_{\text{mix}}|$ *are not independent*. *However, the functional approach allows more general states represented by functionals* $(\rho|$ *for which* $\rho_E\neq\rho_{EE}$, *i.e., states which cannot be represented by normalized vectors or by density operators*. These generalized states are discussed in Sec. II C.

C. Generalized states in the functional approach

The functional approach allows us to have well-defined expressions for *generalized states* that are not defined in the usual formalism.

(i) Consider in the first place the state corresponding to a well-defined value E of the energy. As we have explained, if we represent this state by the generalized eigenvector $|E\rangle$ of the Hamiltonian, $\langle E|E\rangle$ and $\langle E|H|E\rangle$ are not defined. The standard procedure in the usual formalism is to make the spectrum of the Hamiltonian discrete by putting the system in a box where $|E\rangle$ can be normalized, and to make the volume of the box very big after all the relevant calculations.

This is not necessary in the functional approach, where the ''bra'' $(E|$ represent a state with energy E and generalized trace equal to 1: Using Eq. (12) we obtain

$$\langle H^n\rangle=(E|H^n)=(E|\int dE'|E')(E')^n = \int dE'\,\delta(E-E')(E')^n=E^n,$$

from which we easily deduce that the state $(E|$ has a well-defined value E of the energy (i.e., with no deviation from the mean value)

$$\langle H\rangle=(E|H)=E, \quad \langle(H-\langle H\rangle)^n\rangle=(E|(H-\langle H\rangle)^n)=0.$$

For the generalized trace we obtain

$$(E|I)=(E|\int dE'|E')=\int dE'\,\delta(E-E')=1.$$

(ii) As we pointed out in Sec. II A, it is impossible to give a description of the state for $t\to\infty$ using the pure or mixed states of the usual formalism. However, the asymptotic states are well defined in the functional approach.

In the Appendix we prove that if the ''components'' of ρ and O are such that $g_0(E,E')\equiv(\rho_0)^*_{EE'}O_{EE'}$ is a Schwartz function in $[0,\infty)\times[0,\infty)$, the second term of the right-hand side in Eq. (22) vanishes when $t\to\infty$, and therefore we obtain the *weak limit*

$$\lim_{t\to\infty}(\rho_t|O)=(\rho_\infty|O), \quad (\rho_\infty|\equiv\int dE(\rho_0)^*_E(E|. \tag{27}$$

Notice that $(\rho_\infty|$ is neither a pure nor a mixed state, because $(\rho_\infty)_E\neq(\rho_\infty)_{EE'}$, but it is a well-defined state functional with ''trace'' equal to 1 $[(\rho_\infty|I)=1]$.

D. Equilibrium and decoherence

The existence of weak limits for the state functionals when $t\to\infty$ makes this formalism specially suitable to describing the time evolution of decaying quantum systems and the approach to equilibrium in quantum-statistical mechanics. It is also reminiscent of the weak equilibrium limit of mixing classical systems [21].

A standard result of ordinary quantum mechanics is that a pure state (i.e., a state that can be represented by a normalized vector) remains pure during time evolution. However, this is no more valid for weak limits than Eq. (27). The asymptotic form of the state functional obtained for $t\to\infty$ has only diagonal components $[(\rho_\infty)_E\neq 0,\ (\rho_\infty)_{EE'}=0]$. Therefore, ρ_∞ *cannot be represented by a pure or mixed state of the usual formalism*, because if this were the case we should have $(\rho_\infty)_E=(\rho_\infty)_{EE}$. An initially *pure state* with wave function $\langle E|\Psi_0\rangle$ evolves for $t\to\infty$ into a *generalized state* given by the functional

$$(\rho_\infty|=\int dE\langle E|\Psi_0\rangle\langle\Psi_0|E\rangle(E|,$$

in which the generalized states $(E|$ defined above are distributed with probability density $\langle E|\Psi_0\rangle\langle\Psi_0|E\rangle$.

This formalism is an alternative explanation of quantum decoherence, where the usual role of coarse graining is now played out by the fact that the limit is really $(\rho_t|O)\to(\rho_\infty|O)$ *for all observables* $O\in\mathcal{O}$. As these O are all the possible observables, among them we may choose some observables that only take into consideration the states of some subspace of $\mathcal{S}$ (sometimes called the relevant subspace) and neglect the states of the complementary subspace (the irrelevant subspace). In this case we would obtain a coarse-graining formalism. The new formalism avoids the problem of choosing one particular relevant subspace, since it works with *all* possible observables of space $\mathcal{O}$ at the same time. As is well known, decoherence is a very important phenomenon, since it allows the creation of a bridge between quantum and classical mechanics. This is possible since in diagonal matrixes we can use the typical Boolean probability theory of classical physics.[3]

The presence of decoherence shows that we are near the formulation of a time-asymmetric quantum mechanics, but it is not yet so, since really we can repeat the limit (27) for $t\to-\infty$ and we will obtain the same result (as in the mixing classical evolutions). To obtain a real-time asymmetric quantum mechanics we must endow the spaces $\mathcal{O}$ and $\mathcal{S}$ with the time-asymmetric analyticity properties, as we have done in Ref. [20], and as we will see in Sec. IV. In doing so we will solve yet another problem.

III. FRIEDRICHS MODEL

Up to now we have expressed the operators representing observables in terms of $|E)\equiv|E\rangle\langle E|$ and $|EE')\equiv|E\rangle\langle E'|$, $|E\rangle$ ($\langle E|$) being generalized right (left) eigenvectors of the *total* Hamiltonian H of the system. Equations (12) define the corresponding functionals $(E|$ and $(EE'|$ that we can use to expand the states. It is not the usual situation to know the generalized eigenvectors of H. Usually, we just have at our disposal a complete set of generalized eigenvectors of H_0, the *unperturbed* Hamiltonian. This is not only a technical problem of calculation: the eigenvectors of H_0 are usually of practical importance if they are eigenvectors of observables that can be realized in the laboratory. For these reasons it would be convenient (and somehow necessary) to implement the generalized formalism in terms of the eigenvectors of H_0. This will be done in this section for the Friedrichs model.

A. States and observables with diagonal singularity

Let us consider the Friedrichs model, with the Hamiltonian

$$H=H_0+V, \quad H_0=m|1\rangle\langle 1|+\int_0^\infty \omega|\omega\rangle\langle\omega|d\omega,$$

$$V=\int_0^\infty V_\omega[|\omega\rangle\langle 1|+|1\rangle\langle\omega|]d\omega. \tag{28}$$

As $\langle\omega|H|\omega'\rangle=\omega\delta(\omega-\omega')$, there is a diagonal singularity in H. Let us call

$$|1)\equiv|1\rangle\langle 1|, \quad |\omega)\equiv|\omega\rangle\langle\omega|, \quad |\omega\omega')\equiv|\omega\rangle\langle\omega'|,$$

$$|1\omega)\equiv|1\rangle\langle\omega|, \quad |\omega 1)\equiv|\omega\rangle\langle 1|. \tag{29}$$

The form of the Hamiltonian operator given in Eq. (28) suggests that we give the following definition: any element O belonging to the space $\mathcal{O}$ of observables with diagonal singularity can be written as

$$O=O^d+O^c, \quad O^d\equiv O_1|1)+\int O_\omega|\omega)d\omega,$$

$$O^c\equiv\int O_{1\omega'}|1\omega')d\omega'+\int O_{\omega 1}|\omega 1)d\omega$$

$$+\int O_{\omega\omega'}|\omega\omega')d\omega d\omega'. \tag{30}$$

where $O_1=O_1^*$, and $O_\omega=O_\omega^*$, $O_{1\omega}=O_{\omega 1}^*$, $O_{\omega\omega'}=O^*_{\omega'\omega}$ are ordinary functions of the variables ω and ω'. Since H has a diagonal part $H^d=H_0$ of the form given in Eq. (30), H belongs to $\mathcal{O}$.

[3] We will further discuss decoherence using the functional approach elsewhere.

We also assume diagonal singularities in the space of states, which are represented by functionals ρ acting on observables O:

$$(\rho|O)=\rho_1^* O_1+\int d\omega \rho_\omega^* O_\omega+\int d\omega' \rho_{1\omega'}^* O_{1\omega'}$$
$$+\int d\omega \rho_{\omega 1}^* O_{\omega 1}+\int\int d\omega d\omega' \rho_{\omega\omega'}^* O_{\omega\omega'}.$$

For this purpose it is convenient to define a set of functionals $(1|$, $(\omega|$, $(1\omega|$, $(\omega 1|$ and $(\omega\omega'|$ with the following properties [11]:

$$(1|1)=1, \quad (1|\omega)=(1|1\omega)=(1|\omega 1)=(1|\omega\omega')=0,$$
$$(\omega|\omega')=\delta(\omega-\omega'),$$
$$(\omega|1)=(\omega|1\omega')=(\omega|\omega' 1)=(\omega|\omega'\omega'')=0,$$
$$(1\omega|1\omega')=\delta(\omega-\omega'),$$
$$(1\omega|1)=(1\omega|\omega')=(1\omega|\omega' 1)=(1\omega|\omega'\omega'')=0,$$
$$(\omega 1|\omega' 1)=\delta(\omega-\omega'),$$
$$(\omega 1|1)=(\omega 1|\omega')=(\omega 1|1\omega')=(\omega 1|\omega'\omega'')=0,$$
$$(\omega\omega'|\eta\eta')=\delta(\omega-\eta)\delta(\omega'-\eta'),$$
$$(\omega\omega'|1)=(\omega\omega'|\eta)=(\omega\omega'|1\eta)=(\omega\omega'|\eta 1)=0. \tag{31}$$

In terms of these functionals, any element $(\rho|$ of the space $\mathcal{S}$ of states ($\mathcal{S}\subset\mathcal{O}'$) is assumed to have the following form [11]:

$$\rho=\rho^d+\rho^c, \quad \rho^d=\rho_1^*(1|+\int \rho_\omega^*(\omega|d\omega,$$
$$\rho^c=\int \rho_{\omega 1}^*(\omega 1|d\omega+\int \rho_{1\omega'}^*(1\omega'|$$
$$+\int \rho_{\omega\omega'}^*(\omega\omega'|d\omega d\omega', \tag{32}$$

where

$$\rho_1=\rho_1^*\geqslant 0, \ \ \rho_\omega=\rho_\omega^*\geqslant 0, \ \ \rho_{\omega 1}=\rho_{1\omega}^*, \ \ \rho_{\omega\omega'}=\rho_{\omega'\omega}^*, \tag{33}$$

ρ_ω^*, $\rho_{1\omega'}^*$, $\rho_{\omega 1}^*$, and $\rho_{\omega\omega'}^*$ being ordinary functions of the variables ω and ω', and also

$$\rho_1+\int \rho_\omega d\omega=1. \tag{34}$$

Then we will say that $\rho\in\mathcal{S}$.

Equations (33) are the conditions for ρ to be a positive functional, while Eq. (34) is a consequence of the total probability condition

$$(\rho|I)=(\rho|1)+\int d\omega(\rho|\omega)=1, \quad |I)\equiv|1)+\int |\omega)d\omega. \tag{35}$$

The condition $(\rho|I)=1$ on the states can be interpreted as a generalization of the concept of trace, expressing the total probability condition. $(\rho|1)=\rho_1$ is the probability of the state being in the pure state $|1\rangle\langle 1|$ and $(\rho|\omega)=\rho_\omega$ is the probability density of the state being in the pure state $|\omega\rangle\langle\omega|$.

As in the previous section the new formalism contains the usual approach of quantum mechanics. In fact, let us consider a pure state represented by the wave function

$$|\psi\rangle=\psi_1|1\rangle+\int d\omega \psi_\omega|\omega\rangle,$$
$$\langle\psi|\psi\rangle=\psi_1^*\psi_1+\int d\omega \psi_\omega^*\psi_\omega=1. \tag{36}$$

For an observable O, having diagonal singularity as in expression (30), we have

$$\langle\psi|O|\psi\rangle=\psi_1^*\psi_1 O_1+\int d\omega \psi_\omega^*\psi_\omega O_\omega+\int d\omega' \psi_1^*\psi_{\omega'} O_{1\omega'}$$
$$+\int d\omega \psi_\omega^*\psi_1 O_{\omega 1}+\int d\omega d\omega' \psi_\omega^* \ \psi_{\omega'} O_{\omega\omega'}. \tag{37}$$

The mean value (37) of O in the pure state $|\psi\rangle$, can be written as $(\rho_{\text{pure}}|O)$, if we define the functional

$$(\rho_{\text{pure}}|\equiv\psi_1^*\psi_1(1|+\int d\omega \psi_\omega^*\psi_\omega(\omega|+\int d\omega' \psi_1^*\psi_{\omega'}(1\omega'|$$
$$+\int d\omega \psi_\omega^*\psi_1(\omega 1|$$
$$+\int d\omega d\omega' \psi_\omega^* \ \psi_{\omega'}(\omega\omega'|. \tag{38}$$

Acting with $(\rho_{\text{pure}}|$, given in Eq. (38), on an observable $|O)$, given by Eq. (30), we easily prove that $(\rho_{\text{pure}}|O)=\langle\psi|O|\psi\rangle$. Following the arguments of the previous section, it is easy to show that the mixed states of the usual approach can also be represented by a functional acting on the observables with diagonal singularity.

Expressions such as $\langle\omega|\omega\rangle$ or $\langle\omega|H|\omega\rangle$ are not defined. However, the generalized state $(\omega|$ has a well-defined energy and generalized trace, i.e.,

$$\langle I\rangle=(\omega|I)=(\omega|\{|1)+\int d\omega'|\omega')\}=\int d\omega' \delta(\omega-\omega')=1,$$
$$\langle H\rangle=(\omega|H)=(\omega|\{m|1)+\int d\omega' \omega'|\omega')$$
$$+\int d\omega' V_{\omega'}[|1\omega')+|\omega' 1)]=\omega. \tag{39}$$

B. Time evolution and asymptotic states

The time evolution of the states is determined by an operator $\mathbb{U}_t$ acting on ρ, as defined in Eq. (19). We are going to consider observables $O \in \mathcal{O}$, as in Eq. (30), having a diagonal singularity. In addition, we assume, as usual, that O_ω, $O_{\omega 1}$, $O_{1\omega'}$, and $O_{\omega\omega'}$ are regular functions of the variables ω and ω'.

The Lippmann-Schwinger generalized eigenvectors of the Hamiltonian are [14]

$$|\omega^+\rangle = |\omega\rangle + \frac{V_\omega}{\eta_+(\omega)}\left[|1\rangle + \int \frac{d\omega' V_{\omega'}|\omega'\rangle}{\omega-\omega'+i0}\right],$$

$$\langle\omega^+| = \langle\omega| + \frac{V_\omega}{\eta_-(\omega)}\left[\langle 1| + \int \frac{d\omega' V_{\omega'}\langle\omega'|}{\omega-\omega'-i0}\right],$$

$$\eta_\pm(\omega) \equiv \omega - m - \int \frac{d\omega' V_{\omega'}^2}{\omega \pm i0 - \omega'}. \tag{40}$$

If these conditions are fulfilled, it can be proved that the generalized eigenvectors (40) form a complete orthonormal system [14], which we can use to expand the observables. We obtain

$$O = \int d\omega O_\omega^{(+)}|\omega^+\rangle\langle\omega^+| + \int\int d\omega\, d\omega' O_{\omega\omega'}^{(+)}|\omega^+\rangle\langle\omega'^+|. \tag{41}$$

Comparing Eq. (30) with Eq. (41), it is easy to show that

$$O_\omega^{(+)} = O_\omega .$$

The time evolution is given by

$$\begin{aligned}(\rho_t|O) &= (\rho_0|O_t)\\ &= \int d\omega (\rho_0||\omega^+\rangle\langle\omega^+|) O_\omega\\ &\quad + \int d\omega d\omega' (\rho_0||\omega^+\rangle\langle\omega'^+|) e^{i(\omega-\omega')t} O_{\omega\omega'}^{(+)} .\end{aligned} \tag{42}$$

Using the results of the Appendix, the second term goes to zero when $t\to\infty$, and we obtain

$$\lim_{t\to\infty}(\rho_t|O) = (\rho_\infty|O), \quad (\rho_\infty| = \int d\omega (\rho_0||\omega^+\rangle\langle\omega^+|)(\omega|. \tag{43}$$

For the initial condition

$$(\rho_0| = (\rho_0|1)(1| + \int (\rho_0|\omega)(\omega| d\omega,$$

$$(\rho_0|1) + \int (\rho_0|\omega) d\omega = 1,$$

representing a generalized mixture of discrete and continuous modes, we obtain

$$(\rho_\infty| = \int d\omega\left[(\rho_0|1)\frac{V_\omega^2}{\eta_+(\omega)\eta_-(\omega)} + (\rho_0|\omega)\right](\omega|, \tag{44}$$

showing the complete decay of the $(1|$ component of the state,[4] and the simultaneous appearance of an additional part in the diagonal $(\omega|$ component, with a maximum at $\omega = m$. [In fact, it is easy to show that $V_\omega^2/\eta_+(\omega)\eta_-(\omega) \approx \delta(\omega - m)$ for very small V_ω, see Ref. [20], Eq. (80)]. In other words, the unstable state $(1|$ decays in the state of the continuous spectrum, as the electrons decay in the electromagnetic field, giving its energy to the continuous radiation mode corresponding to this energy; a well-established experimental phenomenon, already explained in Ref. [20].

The time evolution for the $(1|$ component of the state is

$$(\rho_t|1) = (\rho_0|1)\int\int d\omega d\omega' e^{i(\omega-\omega')t} \times \frac{V_\omega^2}{\eta_+(\omega)\eta_-(\omega)}\frac{V_{\omega'}^2}{\eta_+(\omega')\eta_-(\omega')}. \tag{45}$$

As is well known, no pure exponential decay is obtained from the previous expression, but it has a dominant exponential behavior. The deviations from this exponential behavior are more important for small times (Zeno effect) and for long times (Khalfin effect).

Now we can see in detail how a pure state becomes a generalized state. For example, the initial state given by the functional $(\rho_0| = (1|$ is a pure state, because it can also be represented by the wave function $|1\rangle$, but the weak limit for $t\to\infty$ of $(\mathbb{U}_t\rho_0|$ is $(\rho_\infty| = \int d\omega [V_\omega^2/\eta_+(\omega)\eta_-(\omega)](\omega|$, which is not a pure state, but a generalized state, where the state $(\omega|$ has probability density $V_\omega^2/\eta_+(\omega)\eta_-(\omega)$. Then, in this way, *it is possible for a pure state to became a generalized one*, and the phenomenon of decoherence is feasible. This nonstandard result suggests that this formalism may be useful for the description of the approach to equilibrium in quantum-statistical mechanics [12].

IV. GENERALIZED COMPLEX SPECTRAL DECOMPOSITION AND TIME EVOLUTION

Equation (42) is an exact expression containing all the information about the time evolution of the Friedrichs model, including the asymptotic state for $t\to\infty$. Nevertheless the evolution can be better visualized using a generalized spectral expansion that allows us to compute the characteristic decaying times of the process. Moreover, to obtain this ex-

[4]The Hamiltonian (28) corresponds to the one excited mode of the Hamiltonian:

$$H = m b^\dagger b + \int d\omega \omega a_\omega^\dagger a_\omega + \int d\omega V_\omega [b^\dagger a_\omega + a_\omega^\dagger b],$$

$$[b,b^\dagger] = 1, \quad [a_\omega, a_{\omega'}^\dagger] = \delta(\omega-\omega').$$

Therefore, the field is at zero temperature and the exited mode $|1\rangle$ decays. This is not the case if the field has an infinite number of exited modes, as we discussed in Ref. [12].

pansion we somehow are forced to introduce time asymmetry into the play.[5]

With the interaction term V of the Hamiltonian (28), the Lippmann-Schwinger solutions (40) form a generalized complete orthonormal system for which the Hamiltonian is given by $H=\int_0^\infty d\omega\omega|\omega^+\rangle\langle\omega^+|$. The discrete eigenvalue m of the Hamiltonian $H_0=m|1\rangle\langle 1|+\int_0^\infty d\omega|\omega\rangle\langle\omega|$ is eliminated from the expansion of H by the interaction. If we consider the analytic extension to the lower half plane of the resolvent of the Hamiltonian, it is possible to show that the simple pole at $z=m$ for the unperturbed case is translated by the interaction with a pole at $z_1=\omega_1-(i/2)\gamma_1\in\mathbb{C}^-$, for which $\eta_+(z_1)=0$. In this subsection we present a generalized spectral decomposition including z_1 and z_1^* as generalized eigenvalues, in order to make explicit the ‘‘pure exponential component’’ of the decay.

Let us first go to the Heisenberg picture and consider the expansion (41) of an observable $O(t)\in\mathcal{O}$, and define the singular invariant (inv) and the regular fluctuating (fluc) parts by

$$O_{\rm inv}\equiv\int d\omega O_\omega^{(+)}|\omega^+\rangle\langle\omega^+|,$$

$$O_{\rm fluc}\equiv O-O_{\rm inv}=\int\int d\omega\, d\omega' O_{\omega\omega'}^{(+)}|\omega^+\rangle\langle\omega'^+| \quad (46)$$

$O_{\rm inv}$ being the invariant part of O under the time evolution ($\mathbb{U}_t^\dagger O_{\rm inv}=O_{\rm inv}$). It can be easily proved using Eqs. (40) that if $O_{\rm fluc}$ is represented in the unperturbed basis ($|1\rangle,|\omega\rangle$), we obtain

$$(O_{\rm fluc})_\omega=0.$$

In what follows we assume that the functions $O_{\omega\omega'}$, $O_{\omega 1}$, and $O_{1\omega'}$ appearing in the expansion (30) of O in the unperturbed basis can be analytically extended to the upper (lower) complex half plane in the variable $\omega(\omega')$. This is an extra condition that we impose on the observables of space $\mathcal{O}$, the one that introduces time asymmetry, and allows us to define a rigging in the theory. (Moreover, if we would like to decompose the evolution group into two semigroups, we may choose the analytic functions in the Hardy classes, as in Ref. [20], but we will discuss this possibility elsewhere.) Our assumption implies that the functions $(O_{\rm fluc})_{\omega\omega'}$, $(O_{\rm fluc})_{\omega 1}$, and $(O_{\rm fluc})_{1\omega'}$ can also be analytically extended to the upper (lower) complex half plane in the variable $\omega(\omega')$. Therefore these analytical properties make it possible to premultiply $O_{\rm fluc}$ by

$$I^\dagger=|\tilde{f}_1\rangle\langle f_1|+\int d\omega|\tilde{f}_\omega\rangle\langle f_\omega|$$

[see Eq. (39) of Ref. [20]] and to postmultiply $O_{\rm fluc}$ by

$$I=|f_1\rangle\langle\tilde{f}_1|+\int d\omega|f_\omega\rangle\langle\tilde{f}_\omega|,$$

[see Eq. (33) of Ref. [20]]. Then

$$O_{\rm fluc}=\left[|\tilde{f}_1\rangle\langle f_1|+\int d\omega|\widetilde{f_\omega}\rangle\langle f_\omega|\right]O_{\rm fluc}\times\left[|f_1\rangle\langle\tilde{f}_1|+\int d\omega|f_\omega\rangle\langle\widetilde{f_\omega}|\right], \quad (47)$$

where [13,15]

$$|\widetilde{f_1}\rangle\equiv\frac{1}{\sqrt{\eta'_-(z_1^*)}}\left[|1\rangle-\int_0^\infty d\omega V_\omega\left(\frac{1}{\omega-s}\right)^-_{z_1^*}|\omega\rangle\right],$$

$$\langle f_1|\equiv\frac{1}{\sqrt{\eta'_-(z_1^*)}}\left[\langle 1|-\int_0^\infty d\omega V_\omega\left(\frac{1}{\omega-s}\right)^-_{z_1^*}\langle\omega|\right],$$

$$|\widetilde{f_\omega}\rangle\equiv|\omega^+\rangle=|\omega\rangle+\frac{V_\omega}{\eta_+(\omega)}\left[|1\rangle+\int_0^\infty\frac{d\omega' V\omega'}{\omega-\omega'+io}|\omega'\rangle\right],$$

$$\langle f_\omega|\equiv\langle\omega|+\frac{V_\omega}{\widetilde{\eta_-(\omega)}}\left[\langle 1|+\int_0^\infty\frac{d\omega' V_{\omega'}}{\omega-\omega'-io}\langle\omega'|\right], \quad (48)$$

$$|f_1\rangle\equiv\frac{1}{\sqrt{\eta'_+(z_1)}}\left[|1\rangle-\int_0^\infty d\omega V_\omega\left(\frac{1}{\omega-s}\right)^+_{z_1}|\omega\rangle\right],$$

$$\langle\widetilde{f_1}|\equiv\frac{1}{\sqrt{\eta'_+(z_1)}}\left[\langle 1|-\int_0^\infty d\omega V_\omega\left(\frac{1}{\omega-s}\right)^+_{z_1}\langle\omega|\right],$$

$$|f_\omega\rangle\equiv\omega\rangle+\frac{V_\omega}{\widetilde{\eta_+(\omega)}}\left[|1\rangle+\int_0^\infty\frac{d\omega' V_{\omega'}}{\omega-\omega'+io}|\omega'\rangle\right],$$

$$\langle\widetilde{f_\omega}|\equiv\langle\omega^+|=\langle\omega|+\frac{V_\omega}{\eta_-(\omega)}\times\left[\langle 1|+\int_0^\infty\frac{d\omega' V_{\omega'}}{\omega-\omega'-io}\langle\omega'|\right]. \quad (49)$$

In the last expressions $z_1\in\mathbb{C}^-$ is the single solution of $\eta_+(z)=0$, $\eta_+(z)$ being the analytic extension to the lower half plane of the function $\eta_+(\omega)$ defined in Eq. (40). In Eqs. (48) and (49) the distributions $[1/(\omega-s)]^+_{z_1}$, $[1/(\omega-s)]^-_{z_1^*}$, $\tilde{\eta}_+(\omega)$, and $\tilde{\eta}_-(\omega)$ are used. They are defined by the equations

$$\int d\omega\left(\frac{1}{\omega-s}\right)^+_{z_1}\varphi(\omega)\equiv\int d\omega\frac{1}{\omega-z_1}\varphi(\omega)+2\pi i\varphi(z_1),$$

$$\int d\omega\left(\frac{1}{\omega-s}\right)^-_{z_1^*}\varphi(\omega)\equiv\int d\omega\frac{1}{\omega-z_1^*}\varphi(\omega)-2\pi i\varphi(z_1^*), \quad (50)$$

[5]For the sake of simplicity the function V_ω is chosen in such a way that $\eta_\pm(\omega)$ does not vanish for any $\omega\in\mathbb{R}^+$ [and also the analytic extension to the lower half complex plane $\eta_+(z)$ of $\eta_+(\omega)$ has just one simple zero at $z=z_1\in\mathbb{C}^-$]

$$\int d\omega \frac{1}{\widetilde{\eta_+(\omega)}} \varphi(\omega) \equiv \int d\omega \frac{1}{\eta_+(\omega)} \varphi(\omega) + 2\pi i \frac{\varphi(z_1)}{\eta'_+(z_1)},$$

$$\int d\omega \frac{1}{\widetilde{\eta_-(\omega)}} \varphi(\omega) \equiv \int d\omega \frac{1}{\eta_-(\omega)} \varphi(\omega) - 2\pi i \frac{\varphi(z_1^*)}{\eta'_-(z_1^*)}. \quad (51)$$

The vectors defined in Eqs. (48) and (49) are generalized eigenvectors of the Hamiltonian, obtained by Petrosky, Prigogine, and Tasaki [13] using a time ordering rule, and previously constructed by Sudarshan, Chiu, and Gorini [14] using analytic continuation techniques. They satisfy the equations

$$\langle \tilde{f}_1 | f_1 \rangle = 1, \quad \langle \widetilde{f_\omega} | f_{\omega'} \rangle = \delta(\omega - \omega'),$$

$$\langle \tilde{f}_1 | f_\omega \rangle = \langle \widetilde{f_\omega} | f_1 \rangle = 0,$$

$$H = z_1 | f_1 \rangle \langle \tilde{f}_1 | + \int d\omega \omega | f_\omega \rangle \langle \widetilde{f_\omega} |, \quad (52)$$

$$\langle f_1 | \tilde{f}_1 \rangle = 1, \quad \langle f_\omega | \widetilde{f_{\omega'}} \rangle = \delta(\omega - \omega'),$$

$$\langle f_1 | \widetilde{f_\omega} \rangle = \langle f_\omega | \tilde{f}_1 \rangle = 0,$$

$$H^\dagger = z_1^* | \tilde{f}_1 \rangle \langle f_1 | + \int d\omega \omega | \widetilde{f_\omega} \rangle \langle f_\omega |. \quad (53)$$

As $\mathbb{U}_t^\dagger O = e^{iH^\dagger t} O e^{-iHt}$ and $O = O_{\text{inv}} + O_{\text{fluc}}$, we obtain

$$\mathbb{U}_t^\dagger O_{\text{inv}} = O_{\text{inv}} = \int d\omega \Pi_\omega O, \quad (54)$$

and

$$\mathbb{U}_t^\dagger O_{\text{fluc}} = e^{iH^\dagger t} O_{\text{fluc}} \, e^{-iHt}$$
$$= \Big\{ e^{i(z_1^* - z_1)t} \Pi_{11} + \int d\omega e^{i(z_1^* - \omega)t} \Pi_{1\omega} + \int d\omega e^{i(\omega - z_1)t} \Pi_{\omega 1} + \int d\omega d\omega' e^{i(\omega - \omega')t} \Pi_{\omega\omega'} \Big\} O, \quad (55)$$

where

$$\Pi_\omega O \equiv | \widetilde{f_\omega} \rangle O_\omega \langle \widetilde{f_\omega} |, \quad \Pi_{11} O \equiv | \tilde{f}_1 \rangle \langle f_1 | O_{\text{fluc}} | f_1 \rangle \langle \widetilde{f_1} |,$$

$$\Pi_{1\omega} O \equiv | \tilde{f}_1 \rangle \langle f_1 | O_{\text{fluc}} | f_\omega \rangle \langle \widetilde{f_\omega} |,$$

$$\Pi_{\omega 1} O \equiv | \widetilde{f_\omega} \rangle \langle f_\omega | O_{\text{fluc}} | f_1 \rangle \langle \widetilde{f_1} |,$$

$$\Pi_{\omega\omega'} O \equiv | \widetilde{f_\omega} \rangle \langle f_\omega | O_{\text{fluc}} | f_{\omega'} \rangle \langle \widetilde{f_{\omega'}} |. \quad (56)$$

Then as $z_1 = \omega_1 - (i/2)\gamma_1$ we conclude that the characteristic decaying times of the four terms in the right-hand side of Eq. (55) are

$$\gamma_1^{-1}, \quad \left(\frac{\gamma_1}{2}\right)^{-1}, \quad \left(\frac{\gamma_1}{2}\right)^{-1}, \quad \infty,$$

respectively. The last (continuous) term has an infinite practical decaying time (if computed in the exponential period), since the interaction couples modes $|1\rangle$ and $|\omega\rangle$ but does not couple the modes of the continuous among themselves.

The time evolution of an observable given by Eqs. (54) and (55), together with Eq. (19) relating Schrödinger and Heisenberg pictures, allow us to obtain our main result, namely, the following expressions for the time evolution of states in the Schrödinger representation:

$$(\rho_t| = (\rho_0| \mathbb{U}_t^\dagger = \int d\omega (\rho_0 | \Pi_\omega + e^{i(z_1^* - z_1)t} (\rho_0| \, \Pi_{11} + \int d\omega e^{i(z_1^* - \omega)t} \, (\rho_0| \, \Pi_{1\omega} + \int d\omega e^{i(\omega - z_1)t} \, (\rho_0| \, \Pi_{\omega 1} + \int d\omega d\omega' e^{i(\omega - \omega')\, t} \, (\rho_0| \Pi_{\omega\omega'} . \quad (57)$$

For the previous expression to be well defined, we need to compute $(\rho_0 || \widetilde{f_\omega} \rangle \langle \widetilde{f_\omega} |)$, $(\rho_0 || \tilde{f}_1 \rangle \langle \tilde{f}_1 |)$, $(\rho_0 || \tilde{f}_1 \rangle \langle \widetilde{f_\omega} |)$, $(\rho_0 || \widetilde{f_\omega} \rangle \langle \widetilde{f_1} |)$, and $(\rho_0 || \widetilde{f_\omega} \rangle \langle \widetilde{f_{\omega'}} |)$. Taking into account Eqs. (48) and (49), we conclude that it is necessary to restrict the space $\mathcal{S} \subset \mathcal{O}'$ of states in such a way that the functions $\rho_{\omega\omega'}^*$, $\rho_{\omega 1}^*$, and $\rho_{1\omega'}^*$ appearing in Eq. (32) have well-defined analytic extensions to the upper (lower) half of the complex plane in the variable $\omega(\omega')$. This is a consequence of the time-asymmetric structure we have added to the space $\mathcal{O}$. The characteristic decaying times are the same as those listed under Eq. (56).

Moreover, the formalism developed in Sec. II gives $(\rho | I)$ as a generalized definition of the trace of states with diagonal singularity, where I is the identity operator. This definition can be used to obtain the generalized trace of the components of the state appearing in Eq. (57). In terms of the Lippmann-Schwinger solutions (40), or the generalized eigenvectors given in Eqs. (48) and (49), the identity operator is

$$I = I_{\text{inv}} = \int d\omega | \omega^+ \rangle \langle \omega^+ |$$

and therefore $I_\omega = 1$ and $I_{\text{fluc}} = 0$. Taking into account that $| \omega^+ \rangle = | \widetilde{f_\omega} \rangle$ and $\langle \omega^+ | = \langle \widetilde{f_\omega} |$, we also have

$$I = \int d\omega | \widetilde{f_\omega} \rangle \langle \widetilde{f_\omega} |.$$

With the definitions (56) of the projectors and the generalized orthogonality conditions given in Eqs. (52) and (53), we obtain

$$(\rho_0|\int d\omega\Pi_\omega I)=(\rho_0|\int d\omega I_\omega|\widetilde{f_\omega}\rangle\langle\widetilde{f_\omega}|)$$

$$=(\rho_0|\int d\omega|\widetilde{f_\omega}\rangle\langle\widetilde{f_\omega}|)=(\rho_0|I)=1,$$

$$(\rho_0|\Pi_{11}I)=(\rho_0||\tilde{f}_1\rangle\langle f_1|I_{\rm fluc}|f_1\rangle\langle\tilde{f}_1|)=0,$$

$$(\rho_0|\Pi_{1\omega}I)=(\rho_0|\Pi_{\omega 1}I)=(\rho_0|\Pi_{\omega\omega'}I)=0. \qquad (58)$$

As we can see, the time-independent part $(\rho_0|\int d\omega\Pi_\omega$ of the state contains all the generalized trace of $(\rho_t|$, while the time-dependent components have zero trace. This is consistent with the conservation of the trace by time evolution. Moreover, these results also tell us that the time evolving part $(\rho_0|\{\mathbb{I}-\int d\omega\Pi_\omega\}$ cannot be considered a physical state; it is just a fluctuation around the time-independent part $(\rho_0|\int d\omega\Pi_\omega$. All these results coincide with those already obtained in Ref. [20] for the pure-state case.

Even more generally, for any observable Q commuting with the Hamiltonian H, we can write

$$Q=\int d\omega Q_\omega|\omega^+\rangle\langle\omega^+|=\int d\omega Q_\omega|\widetilde{f_\omega}\rangle\langle\widetilde{f_\omega}|; \qquad (59)$$

therefore $Q_{\rm fluc}=0$, and

$$(\rho_0|\int d\omega\Pi_\omega Q)=(\rho_0|Q),$$

$$(\rho_0|\Pi_{11}Q)=(\rho_0|\Pi_{1\omega}\ Q)=(\rho_0|\Pi_{\omega 1}Q)=(\rho_0|\Pi_{\omega\ \omega'}\ Q)=0, \qquad (60)$$

which is consistent with $(\rho_t|Q)=(\rho_0|Q)$. Then the observables that commute with H are not only constants of motion, but their ''fluctuation components'' are just fluctuations around the time-independent part $(\rho_0|Q)$, since their mean values vanish. This conclusion is, of course, also valid for $Q=H$.

So $(\rho_0|\Pi_{11}$, $(\rho_0|\Pi_{1\omega}$, $(\rho_0|\Pi_{\omega 1}$, and $(\rho_0|\Pi_{\omega\omega'}$ (namely, the generalized left eigenvectors of the Liouville operator $\mathbb{L}^\dagger$ with eigenvalues $z_1^*-z_1$, $z_1^*-\omega$, $\omega-z_1$, and $\omega-\omega'$) have no trace, no energy, and the zero mean value of any observable that commutes with H. Therefore these eigenvectors, as any fluctuation, cannot be considered alone as physical states.

Finally the formalism presented in Sec. II for states and observables with diagonal singularity, applied to the Friedrichs model in Liouville space, shows that there is no place for physical states with pure exponential decay. However, the pure exponential decay appears for physical states as an approximation when the interaction V is very small. In this case, using the results of Ref. [20], we obtain the following *weak limits* for the projectors defined in Eq. (56)

$$\lim_{V\to 0}\Pi_\omega=|\omega)(\omega|+|1)\delta(\omega-m)(\omega|,$$

$$\lim_{V\to 0}\Pi_{11}=|1)(1|-|1)(\omega=m|,$$

$$\lim_{V\to 0}\Pi_{1\omega}=|1\omega)(1\omega|, \quad \lim_{V\to 0}\Pi_{\omega 1}=|\omega 1)(\omega 1|,$$

$$\lim_{V\to 0}\Pi_{\omega\omega'}=|\omega\omega')(\omega\omega'|. \qquad (61)$$

Moreover, for small V, $z_1\cong m-i\pi V_m^2$ is an approximated solution of $\eta_+(z_1)=0$, and the weak limits (61) for the projectors can be used in Eq. (57) to obtain

$$\begin{aligned}(\rho_t|\cong&\int d\omega(\rho_0|\omega)(\omega|+e^{-2\pi V_m^2 t}(\rho_0|1)\ (1|\\&+\{1-e^{-2\pi V_m^2 t}\}(\rho_0|1)(m|\\&+\int d\omega e^{-2\pi V_m^2 t}e^{i(m-\omega)\ t}(\rho_0|1\omega)\ (1\omega|\\&+\int d\omega e^{-2\pi V_m^2 t}\ e^{i(\omega-m)\ t}(\rho_0|\omega 1)(\omega 1|\\&+\int d\omega\int d\omega'\ e^{i(\omega-\omega')t}(\rho_0|\omega\omega')\ (\omega\ \omega'|.\end{aligned} \qquad (62)$$

The first three terms in the previous equation give the time evolution of the diagonal part of the state. The discrete mode $(1|$ has an exponential decay, and simultaneously there is a growing part in the continuum with $\omega=m$. There is also a continuum time-independent part, keeping the memory of the initial condition. But here the pure exponential decay is just an approximation.

The last three terms in Eq. (62) give the time evolution of the nondiagonal part of the state. The $(\omega 1|$ and $(1\omega|$ components have exponential decay together with an oscillating factor. There is no exponential decay for the $(\omega\omega'|$ component for the reasons we have already explained below in Eq. (56), but this term gives a vanishing contribution to the mean value of observables for $t\to\infty$ due to the oscillating factor $e^{i(\omega-\omega')t}$.

Then we obtain the *weak* limit

$$\lim_{t\to\infty}(\rho_t|\cong\int d\omega(\rho_0|\omega)(\omega|+(\rho_0|1)(\omega=m|. \qquad (63)$$

The previous approximated expression coincides with the exact expression (44) for small V.

V. CONCLUSIONS

We have applied the formalism of quantum theory of Refs. [9–11] to a simple ''toy'' model with Hamiltonian

$$H=\int_0^\infty dE E|E\rangle\langle E|. \qquad (64)$$

For this system we defined the class $\mathcal{O}$ of observables with diagonal singularity

$$|O)=\int dE O_E|E)+\int\int dE dE' O_{E\ E'}|EE'),$$

$$O\in\mathcal{O}, \quad |E)\equiv|E\rangle\langle E|, \quad |EE')\equiv|E\rangle\langle E'|, \qquad (65)$$

and the class of states $\mathcal{S}\subset\mathcal{O}'$ of the form

$$(\rho|=\int dE\rho_E^*(E|+\int\int dE\, dE'\ \rho_{EE'}^*(E\ E'|, \quad (66)$$

where

$$(E|O)=O_E,\quad (EE'|O)=O_{EE'}. \quad (67)$$

In this formalism we can represent the following.

(i) A *pure state*, i.e., a state that in the usual approach is represented by a normalized vector $|\Psi\rangle=\int dE|E\rangle\langle E|\Psi\rangle$. In the functional approach this state is represented by a functional of the form (66) with

$$\rho_E^*=\langle\Psi|E\rangle\langle E|\Psi\rangle,\quad \rho_{EE'}^*=\langle\Psi|E\rangle\langle E'|\Psi\rangle. \quad (68)$$

(ii) A *mixed state*, i.e., a state that in the usual approach is represented by a mixture of normalized vectors $|\Psi^{(\alpha)}\rangle$ with probabilities $p^{(\alpha)}$. In the functional approach this state is given by a functional of the form (66) with

$$\rho_E^*=\sum_\alpha p^{(\alpha)}\langle\Psi^{(\alpha)}|E\rangle\langle E|\Psi^{(\alpha)}\rangle,$$

$$\rho_{EE'}^*=\sum_\alpha p^{(\alpha)}\langle\Psi^{(\alpha)}|E\rangle\langle E'|\Psi^{(\alpha)}\rangle. \quad (69)$$

(iii) A *generalized state* of the form given in Eq. (66) with $\rho_E^*\neq\rho_{EE'}^*$. The state $(\tilde{E}|$, with energy $\tilde{E}$ is a generalized state, as we have in this case $\rho_E^*=\delta(E-\tilde{E})$ and $\rho_{EE'}^*=0$. Another example of a generalized state is the weak limit for $t\to\infty$ of an initially pure state, given by

$$(\rho_\infty|=\int dE\langle E|\Psi_0\rangle\langle\Psi_0|E\rangle(E|. \quad (70)$$

This result also shows the possibility for a pure state to become a generalized state for very big times.

We also applied the functional approach to the Friedrichs model, with Hamiltonian

$$H=m|1\rangle\langle 1|+\int_0^\infty\omega|\omega\rangle\langle\omega|d\omega+\int_0^\infty V_\omega[|\omega\rangle\langle 1|$$
$$+|1\rangle\langle\omega|]d\omega. \quad (71)$$

In this case, we considered the space $\mathcal{O}$ of observables with diagonal singularity

$$|O)=O_1|1)+\int O_\omega|\omega)\ d\omega+\int O_{1\,\omega'}|1\omega')\ d\omega'$$
$$+\int O_{\omega 1}|\omega 1)\ d\omega+\int O_{\omega\ \omega'}|\omega\omega')d\omega\ d\omega',$$
$$O\in\mathcal{O},$$
$$|1)\equiv|1\rangle\langle 1|,\quad |\omega)\equiv|\omega\rangle\langle\omega|,\quad |\omega\omega')\equiv|\omega\rangle\langle\omega'|,$$
$$|1\omega)\equiv|1\rangle\langle\omega|,\quad |\omega 1)\equiv|\omega\rangle\langle 1|, \quad (72)$$

and the class of states $\mathcal{S}\subset\mathcal{O}'$ of the form

$$(\rho|=\rho_1^*(1|+\int\rho_\omega^*(\omega|d\omega+\int\rho_{\omega 1}^*(\omega 1|d\omega$$
$$+\int\rho_{1\omega'}^*(1\omega'|+\int\rho_{\omega\omega'}^*(\omega\omega'|d\omega d\omega',\quad \rho\in\mathcal{S},$$
$$(1|O)=O_1,\quad (\omega|O)=O_\omega,\quad (\omega 1|O)=O_{\omega 1},$$
$$(1\omega'|O)=O_{1\omega'},\quad (\omega\omega'|O)=O_{\omega\omega'}. \quad (73)$$

We obtained exact expressions for the time evolution of any state functional. For example, we can consider the initial state $(\rho_0|=(1|$, which is a pure state, as it can be represented by the normalized vector $|1\rangle$ in the usual approach. For $t\to\infty$ this state evolves into

$$(\rho_\infty|=\int d\omega\frac{V_\omega^2}{\eta_+(\omega)\eta_-(\omega)}(\omega|. \quad (74)$$

This is a generalized state where the states $(\omega|$ have probability density $V_\omega^2/\eta_+(\omega)\eta_-(\omega)$. For small interaction parameter, this probability density is a sharp peak centered in the value $\omega=m$, corresponding to the unperturbed energy of the decaying state $(1|$.

The ''final'' state given in Eq. (74) is invariant under time inversion and also invariant under time evolution. Then the formalism itself makes evident the intrinsic irreversibility of the decay process.

The generalized state $(\omega|$ has well-defined energy and generalized trace in this formalism, i.e.,

$$\langle H\rangle=(\omega|H)=\omega,\quad \langle I\rangle=(\omega|I)=1.$$

The exact expressions we obtained for the time evolution show that it is impossible to have pure exponential decays. However, the decay of the state $(1|$ deviates from the exponential only for small and large values of time (Zeno and Khalfin effects). Therefore, it is useful to obtain spectral decompositions including the contributions of the single pole at z_1 of the analytic extension to the lower half plane of the S matrix. This spectral decomposition is possible if we consider the observables $O\in\mathcal{O}$ and states $\rho\in\mathcal{S}\subset\mathcal{O}'$ for which the nondiagonal components $O_{\omega 1}$, $O_{1\omega'}$, $O_{\omega\omega'}$, $\rho_{\omega 1}^*$, $\rho_{1\omega'}^*$, and $\rho_{\omega\omega'}^*$ in the unperturbed basis are ordinary functions that can be analytically extended to the upper (lower) complex half plane for the variable ω (ω').

For the Friedrichs model we obtained a generalized spectral decomposition of the form

$$(\rho_t|=(\rho_0|\mathbb{U}_t^\dagger,$$

$$\mathbb{U}_t^\dagger=\int d\omega\Pi_\omega+e^{i(z_1^*-z_1)t}\Pi_{11}+\int d\omega\ e^{i(z_1^*-\omega)t}\Pi_{1\omega}$$
$$+\int d\omega\ e^{i(\omega-z_1)\ t}\ \Pi_{\omega 1}+\int d\omega\ d\omega' e^{i(\omega-\omega')t}\Pi_{\omega\ \omega'}.$$

We proved that $(\rho_0|\Pi_{11}$, $(\rho_0|\Pi_{1\omega}$, $(\rho_0|\Pi_{\omega 1}$, and $(\rho_0|\Pi_{\omega\omega'}$ are generalized left eigenvectors of the Liouville–Von Newmann operator $\mathbb{L}^\dagger$ with eigenvalues $z_1^*-z_1$, $z_1^*-\omega$, $\omega-z_1$, and $\omega-\omega'$, and they have no trace, no energy, and zero mean value of any observable commuting with H.

Therefore these eigenvectors, as any fluctuation, cannot be considered alone as physical states.

There is no place in this formalism for physical states with pure exponential decay. However, we recover the pure exponential decay of the unstable state as an approximation for small interactions, i.e.,

$$(\rho_t| \cong \int d\omega(\rho_0|\omega)(\omega| + e^{-2\pi V_m^2 t}(\rho_0|1)\ (1|$$
$$+\{1-e^{-2\pi V_m^2 t}\}(\rho_0|1)(m|$$
$$+\int d\omega e^{-2\pi V_m^2 t} e^{i(m-\omega)\ t}(\rho_0|1\omega)\ (1\omega|$$
$$+\int d\omega e^{-2\pi V_m^2 t}\ e^{i(\omega-m)\ t}(\rho_0|\omega 1)(\omega 1|$$
$$+\int d\omega \int d\omega' e^{i(\omega-\omega')t}(\rho_0|\omega\omega')\ (\omega\omega'|.$$

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APPENDIX: VANISHING OF THE NONDIAGONAL PARTS OF MEAN VALUES FOR T→∞

In this section we give the conditions under which the limits for $t\rightarrow\infty$ in expressions (4) and (22) give the results of Eqs. (5) and (27). The proof follows the arguments of Ref. [22]. Let us start, considering the expression

$$I(\lambda)=\int_{\mathcal{D}} d\overline{x} g_0(\overline{x})\exp[\lambda\phi(\overline{x})], \tag{A1}$$

where $\mathcal{D}$ is a subset of $\mathbb{R}^n$, ϕ, and g_0 are differentiable functions in $\mathcal{D}$, and λ is a complex parameter.

Provided $\overline{\nabla}\cdot\phi\neq 0$ we can easily prove the following identity:

$$g_0(\overline{x})e^{\lambda\phi(\overline{x})}=\frac{1}{\lambda}\overline{\nabla}\cdot(\overline{H}_0(\overline{x})e^{\lambda\phi(\overline{x})})-\frac{1}{\lambda}(\overline{\nabla}\cdot\overline{H}_0(\overline{x}))e^{\lambda\phi(\overline{x})}, \tag{A2}$$

where

$$\overline{H}_0(\overline{x})\equiv g_0(\overline{x})\frac{\overline{\nabla}\phi(\overline{x})}{|\overline{\nabla}\phi(\overline{x})|^2}, \tag{A3}$$

and therefore

$$I(\lambda)=\frac{1}{\lambda}\int_{\mathcal{P}} e^{\lambda\phi}\overline{H}_0\cdot\overline{N}ds-\frac{1}{\lambda}\int_{\mathcal{D}} e^{\lambda\phi}(\overline{\nabla}\cdot\overline{H}_0)d\overline{x}, \tag{A4}$$

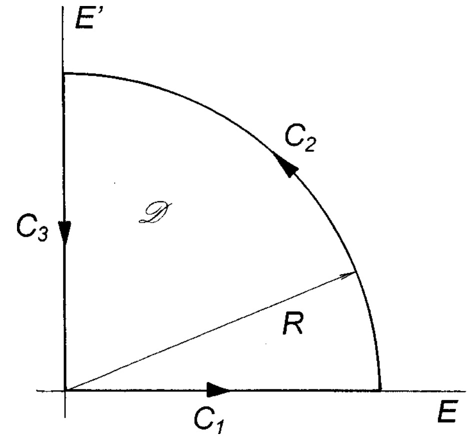

FIG. 1. Domain and boundary for Eq. (A6).

where $\mathcal{P}$ is the boundary of $\mathcal{D}$ with exterior normal $\overline{N}$. In our case we need to compute

$$F(t)=\int_0^\infty dE\int_0^\infty dE'\rho^*_{EE'}O_{EE'}e^{i(E-E')t}, \tag{A5}$$

which is Eq. (A1) with

$$\lambda=it,\quad \overline{x}=(E,E'),\quad \mathcal{D}=[0,\infty)\times[0,\infty),$$

$$\phi(E,E')=E-E',\quad g_0(E,E')=\rho^*_{EE'}O_{EE'},$$

and therefore

$$\overline{\nabla}\cdot\phi=(1,-1),\quad \overline{H}_0=\frac{1}{2}g_0(E,E')(1,-1),$$

$$\overline{\nabla}\cdot\overline{H}_0=\frac{1}{2}(1,-1)\cdot\overline{\nabla}g_0(E,E').$$

The bidimensional domain $\mathcal{D}$ and the boundary $\mathcal{P}$ are represented in Fig. 1, with $\mathcal{P}=C_1+C_2+C_3$, for some $R\gg 1$.

Using Eq. (A4) we obtain

$$2itF(t)=\int_0^\infty dE g_0(E,0)e^{iEt}+\lim_{R\to\infty}\int_{C_2} dl e^{i(E-E')t}g_0(E,E')$$
$$\times(1,-1)\cdot\overline{N}+\int_0^\infty dE' g_0(0,E')e^{-iE't}$$
$$-\lim_{R\to\infty}\int\int_{\mathcal{D}} dE dE' e^{i(E-E')t}$$
$$\times\left(\frac{\partial}{\partial E}-\frac{\partial}{\partial E'}\right)g_0(E,E'). \tag{A6}$$

If $g_0(E,E')=\rho^*_{EE'}O_{EE'}$ is a Schwartz function in $[0,\infty)\times[0,\infty)$, the modulus of the right-hand side of the previous expression is a bounded function of t, and therefore

$$\lim_{t\to\infty}F(t)=0.$$

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